Essentials of Chemistry 3:
Ionic and Covalent Bonding

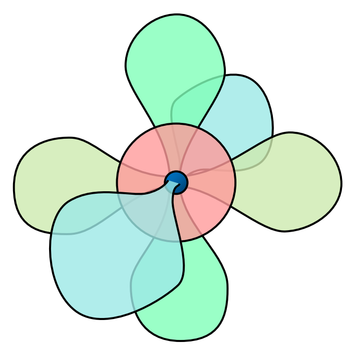
Atoms are at their most stable when the least energy is required to keep them in whatever state they're in, and the states that take the least energy are ones where their orbitals are collectively completely full or completely empty (or, in a pinch, exactly half full), or in other words all the similar orbitals have the same number of electrons in them.

In ionic bonds, atoms stabilize themselves by giving away or taking on extra electrons to round themselves up or down to a full orbital. Sodium has full orbitals plus one extra electron; chlorine is one electron short of a full orbital. We see a solution here: sodium gives its extra one away to a chlorine, and everyone is happy. Each atom has just formed an **ion** (since its electrons no longer balance the charges in their nuclei), and this is **ionic bonding**.

The other solution is **covalent bonding**. No matter which theory of intramolecular bonding you're working with, the **valence electrons** (the electrons in the outermost shell) all stay with their atoms, but they rearrange themselves so that the spaces they occupy overlap each other, allowing the electrons in those spaces to grant that same kind of stability to their atoms without needing to give or take electrons.

ATOMIC STRUCTURE

Let's look at a molecule of oxygen, O_2. In an oxygen atom, the electrons occupy spaces around the nucleus in predictable regions called **orbitals**. Each one is labelled with a number and a letter. The letter tells you which shape: an s orbital is a sphere centered on the nucleus; a p orbital is a dumbbell-shaped space with its thinnest part near the nucleus and two fat spaces pointing in opposite directions, and so on. The number is an energy level number: the bigger the number, the bigger the size of the orbital, so a 1s electron is close to the nucleus; a 2s electron is in a spherical space that's larger, and is far less likely to appear in the space we've already called 1s, and so on.



There are eight protons (positive charges) in the oxygen atom's nucleus so it will naturally come with eight electrons. They'll fill their orbitals from most stable to least stable: two in 1s, two in 2s, and the remaining four in 2p orbitals. There are always three p orbitals at any given energy level and every orbital holds two electrons, so there's room for six electrons in 2p. An oxygen atom is unstable all by itself: the p orbitals are not all empty, full, or half empty. Donating electrons to another oxygen atom will not fix this problem; if one oxygen atom gives away two 2p electrons to fill another atom's orbitals, it will have only two left, which isn't any better. Since we know that O_2 molecules do exist, we need a different model for its structure.

The Lewis structure for oxygen tells us that there is a double bond in the molecule. The simpler **hybridization/VSEPR model** for molecular structure explains that double bond this way: To keep an electron in a 2s orbital takes slightly less energy than it takes to keep an electron in a 2p orbital — that's why we fill the 2s orbital first. The electrons in the 2p orbitals spread out as

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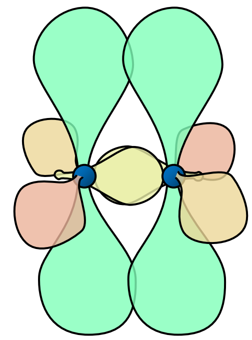
much as possible, putting one electron in each of the three before any of them gets a second one. Those three are equally easy to fill, but the negatively charged electrons want to get as far away from each other as they can be. If we extend these ideas (equal orbitals spread electrons out) to include the 2s orbitals, there's a solution to how an O_2 molecule can exist.



In each oxygen atom, one 2p orbital stays as it is. The atoms are close enough that their 2p orbitals overlap to form a **π bond (pi bond)**. The remaining two 2p orbitals and the 2s orbital in each atom blend together to form three hybridized $2sp^2$ orbitals. (The name tells us what the hybridized orbitals are made from: from energy level **2**, one **s** and **2** **p** orbitals.) The amount of energy it takes to keep an electron in the new orbitals is the same for each, and it's between 2s and 2p. The shape is an exaggerated dumbbell, with one side much larger than the other. These shapes still want to spread out, and the configuration that keeps the electrons as far away from each other (and the untouched 2p orbital) is to form a flat propeller shape with three blades, perpendicular to the line passing through the centre of the 2p orbital and the nucleus, as in the diagram. Two of the new hybridized orbitals, one from each atom, will also overlap, and together they form a **σ bond (sigma bond)**.

This arrangement follows all the rules. The lowest-energy orbitals at energy level 2 are the three $2sp^2$ orbitals. They should fill first, and like all orbitals, they have room for two electrons each. There were six total electrons in the 2s and 2p orbitals before they hybridized, so we need spaces for those six electrons. Two electrons will go into the two orbitals that don't overlap (creating **lone pairs**) which accounts for four of the six. One more can go into the sp^2 orbital that overlaps with its neighbour, and that neighbour atom will put one in at the same time, filling the orbital. We have one more electron to place, but there's no more room in the sp^2 orbitals, so we move on to the orbitals with the next higher energy, which is the unhybridized 2p orbital. The last electron goes there, and the neighbour's last electron does too, and because they overlap, the "pi orbital" is also full. All the orbitals at energy level 2 are full, resulting in a stable molecule.

When a molecule has a single bond between two atoms, it's always a σ bond. If there is a double or triple bond, the "extra" bonds are always π bonds made from unhybridized, overlapping p orbitals, since that's the only way to have a second or third space where this overlap can occur, allowing atoms to share more than one electron. In something like a water molecule, where the oxygen atom will need to share electrons with two distinct hydrogen atoms, all the s and p orbitals will hybridize (allowing all of them to fill from the start), and two separate σ bonds will form. The configuration of orbitals that keeps them as far away from each other as possible is a tetrahedral shape (a three-sided pyramid) and the angle between the orbitals is close to the observed bond angle in a water molecule.